



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:39 PM UTC

PDB ID : 6ZQK / pdb_00006zqk
Title : HER2-binding scFv-Fab fusion 841
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Deposited on : 2020-07-09
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

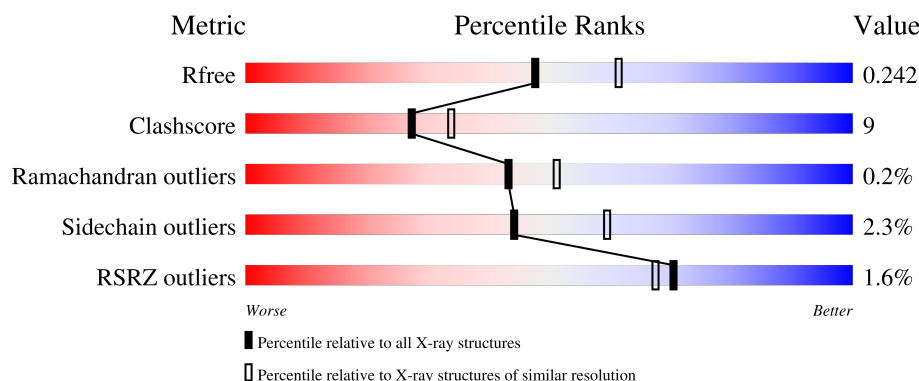
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	469	<div> <div>2%</div> <div>78% 15% 6%</div> </div>
1	C	469	<div> <div>2%</div> <div>74% 19% 6%</div> </div>
2	B	223	<div> <div>2%</div> <div>81% 14% . .</div> </div>
2	D	223	<div> <div>2%</div> <div>77% 18% .</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20423 atoms, of which 9893 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

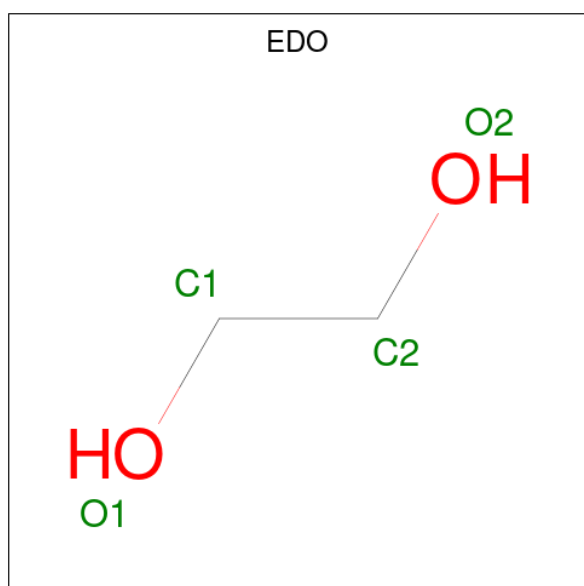
- Molecule 1 is a protein called 841 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	H	N	O	S	0	0	0
			6767	2170	3327	582	677	11			
1	C	443	Total	C	H	N	O	S	0	7	0
			6852	2196	3364	595	686	11			

- Molecule 2 is a protein called 841 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	215	Total	C	H	N	O	S	0	0	0
			3194	1029	1566	267	325	7			
2	D	213	Total	C	H	N	O	S	0	3	0
			3209	1036	1570	267	329	7			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



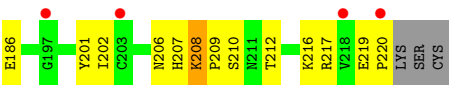
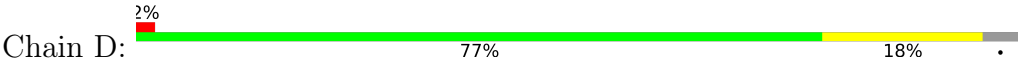
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	56	Total O 56 56	0	0
4	C	97	Total O 97 97	0	0
4	D	48	Total O 48 48	0	0



● Molecule 2: 841 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.08Å 75.64Å 88.60Å 103.56° 90.33° 107.13°	Depositor
Resolution (Å)	48.69 – 2.20 48.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.69-2.20) 92.1 (48.69-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.202 , 0.241 0.204 , 0.242	Depositor DCC
R_{free} test set	2870 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20423	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/3522	0.46	1/4786 (0.0%)
1	C	0.20	0/3584	0.43	0/4868
2	B	0.21	0/1668	0.45	0/2272
2	D	0.21	0/1680	0.51	0/2290
All	All	0.20	0/10454	0.46	1/14216 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	177	ASN	N-CA-CB	-6.27	99.89	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	VAL	Peptide
1	C	176	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	3327	3334	56	3
1	C	3488	3364	3361	79	1
2	B	1628	1566	1573	17	2
2	D	1639	1570	1573	33	3
3	A	20	30	30	3	0
3	C	16	24	24	1	1
3	D	8	12	12	1	0
4	A	90	0	0	14	0
4	B	56	0	0	4	0
4	C	97	0	0	13	0
4	D	48	0	0	10	0
All	All	10530	9893	9907	184	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLY:O	4:C:601:HOH:O	1.66	1.12
1:C:451:HIS:O	1:C:473:ARG:NH1	1.94	1.00
1:C:250:LYS:NZ	4:C:605:HOH:O	1.99	0.96
2:D:133:PRO:O	4:D:402:HOH:O	1.87	0.93
1:C:449:GLU:OE1	1:C:473:ARG:NE	2.02	0.92
2:D:46:GLU:OE1	4:D:401:HOH:O	1.87	0.91
1:C:257:ASP:OD2	4:C:602:HOH:O	1.88	0.91
2:B:46:GLU:OE1	4:B:301:HOH:O	1.88	0.90
1:A:367:GLU:OE1	1:A:435:TYR:OH	1.93	0.86
2:D:165:ALA:O	4:D:403:HOH:O	1.94	0.84
2:D:167:THR:N	4:D:403:HOH:O	2.10	0.82
1:C:74:THR:O	4:C:604:HOH:O	1.98	0.81
1:A:148:ASP:N	1:A:148:ASP:OD1	2.13	0.81
1:A:149:ILE:O	1:A:244:THR:HG21	1.82	0.80
1:C:159:SER:OG	4:C:603:HOH:O	1.97	0.80
2:B:181:GLY:O	4:B:302:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLN:NE2	4:A:608:HOH:O	2.16	0.77
1:A:171:ARG:HD2	4:A:613:HOH:O	1.84	0.77
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.66	0.77
1:A:187:PRO:O	4:A:601:HOH:O	2.05	0.74
1:C:82:GLN:NE2	4:C:610:HOH:O	2.19	0.74
2:D:65:GLN:O	4:D:404:HOH:O	2.05	0.73
2:B:39:GLU:OE1	4:B:303:HOH:O	2.08	0.71
1:C:182:TRP:CD1	1:C:195:ILE:HD11	2.25	0.71
1:C:385:GLU:N	1:C:385:GLU:OE2	2.24	0.70
2:D:167:THR:HG22	4:D:403:HOH:O	1.90	0.70
1:A:11:LEU:HD11	1:A:119:SER:HB3	1.74	0.70
1:A:14:PRO:HG3	1:A:120:SER:HA	1.73	0.69
1:C:261:THR:O	4:C:607:HOH:O	2.11	0.68
2:D:210:SER:HG	2:D:212:THR:HG1	1.42	0.67
1:C:269:VAL:HG22	1:C:340:LEU:HD22	1.76	0.67
1:C:452:LYS:HA	1:C:473:ARG:HH12	1.59	0.67
2:D:181:GLY:O	4:D:406:HOH:O	2.12	0.67
2:B:62:GLN:HG2	4:B:310:HOH:O	1.94	0.66
1:A:151:MET:O	4:A:604:HOH:O	2.13	0.66
1:A:426:THR:O	4:A:603:HOH:O	2.13	0.66
2:D:39:GLU:OE2	4:D:405:HOH:O	2.12	0.66
1:A:318:SER:O	4:A:605:HOH:O	2.14	0.65
1:C:149:ILE:HD12	1:C:240:THR:HG22	1.76	0.65
2:D:157:VAL:HG13	2:D:206:ASN:O	1.97	0.65
1:A:171:ARG:O	4:A:606:HOH:O	2.15	0.65
1:A:179:ALA:HB3	1:A:239:TYR:HB2	1.79	0.65
1:A:23:ALA:O	4:A:607:HOH:O	2.15	0.63
2:D:202:ILE:CD1	2:D:217:ARG:HG2	2.28	0.63
1:C:395:LYS:NZ	1:C:440:THR:OG1	2.22	0.62
1:C:232:THR:OG1	4:C:606:HOH:O	2.10	0.62
2:D:210:SER:OG	2:D:212:THR:OG1	2.17	0.62
1:A:149:ILE:HD12	1:A:240:THR:HG22	1.81	0.61
1:A:317:LYS:NZ	2:B:108:ASP:OD2	2.28	0.61
1:A:206:PRO:HD3	3:A:502:EDO:H12	1.81	0.61
1:C:41:PRO:O	4:C:609:HOH:O	2.16	0.60
2:D:202:ILE:HD12	2:D:217:ARG:HG2	1.84	0.59
1:A:150:GLN:HB2	1:A:173:SER:HB3	1.85	0.58
1:C:186:LYS:NZ	4:C:617:HOH:O	2.36	0.58
2:B:132:ALA:HA	2:B:218:VAL:HG12	1.86	0.58
1:C:451:HIS:C	1:C:473:ARG:HH12	2.09	0.58
1:C:179:ALA:HB3	1:C:239:TYR:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLY:O	1:C:216:THR:HG22	2.03	0.57
1:C:452:LYS:HA	1:C:473:ARG:NH1	2.20	0.56
2:D:11:VAL:HG21	2:D:154:PRO:HG3	1.87	0.56
1:C:184:GLN:HB2	1:C:194:LEU:HD11	1.87	0.56
1:A:105:TYR:HD2	1:A:238:HIS:O	1.89	0.55
1:C:278[B]:ASN:ND2	1:C:333:PHE:O	2.40	0.55
1:A:269:VAL:HG22	1:A:340:LEU:HD22	1.88	0.55
1:C:395:LYS:HZ2	2:D:186:GLU:CD	2.15	0.55
1:A:176:VAL:HG12	1:A:239:TYR:HB3	1.89	0.55
1:C:99:TRP:CE3	1:C:99:TRP:HA	2.41	0.54
1:C:448:TYR:HA	1:C:454:TYR:OH	2.08	0.54
1:A:295:LEU:HD22	1:A:351:GLN:O	2.09	0.53
1:C:47:TRP:CZ3	1:C:242:PRO:HB3	2.43	0.53
1:A:299:GLN:HB2	1:A:309:LEU:HD11	1.91	0.53
1:C:29:ILE:HD12	1:C:53:PRO:CG	2.38	0.53
1:C:408:VAL:HG22	1:C:458:VAL:HG22	1.91	0.53
1:A:99:TRP:NE1	4:A:602:HOH:O	2.12	0.52
2:D:175:ALA:HA	2:D:185:LEU:HB3	1.91	0.52
1:A:151:MET:HB3	1:A:170:CYS:SG	2.50	0.52
1:C:411:LYS:HE3	1:C:416:LEU:HD13	1.92	0.51
1:A:241:THR:HG23	1:A:243:PRO:HD3	1.92	0.51
1:C:1:GLU:HG3	1:C:1:GLU:O	2.11	0.51
1:C:299:GLN:HB2	1:C:309:LEU:HD11	1.91	0.51
1:C:55:ASN:CG	4:C:608:HOH:O	2.53	0.50
1:C:395:LYS:HD3	1:C:440:THR:OG1	2.10	0.50
1:A:153:GLN:HG3	1:A:235:CYS:SG	2.51	0.50
1:C:441:LEU:HD21	1:C:443:LEU:HD11	1.94	0.50
2:D:67:ARG:HG2	2:D:84:SER:O	2.12	0.50
1:C:395:LYS:HZ3	1:C:440:THR:HG1	1.51	0.49
2:D:201:TYR:O	2:D:202:ILE:HD13	2.12	0.49
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.45	0.49
1:C:241:THR:HG23	1:C:242:PRO:HA	1.93	0.49
1:C:99:TRP:HA	1:C:99:TRP:HE3	1.78	0.49
1:C:290:ASN:HD22	3:C:502:EDO:H12	1.78	0.48
2:B:176:VAL:O	2:B:178:GLN:NE2	2.46	0.48
1:C:216:THR:HG23	1:C:216:THR:O	2.13	0.48
1:C:2:VAL:HG13	1:C:109:TYR:CE2	2.48	0.48
1:A:239:TYR:C	4:A:631:HOH:O	2.57	0.48
2:B:100:GLY:HA3	2:B:104:GLU:O	2.14	0.48
2:D:166:LEU:CA	4:D:403:HOH:O	2.62	0.48
1:A:280:ARG:HA	1:A:331:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LYS:HD2	1:C:453:VAL:HG23	1.96	0.47
1:A:452:LYS:O	1:A:472:ASN:O	2.32	0.47
1:C:99:TRP:CZ3	1:C:107:MET:HG3	2.49	0.47
1:A:105:TYR:HB3	1:A:238:HIS:HB2	1.96	0.47
2:D:36:TRP:CE2	2:D:81:MET:HB2	2.50	0.47
2:D:201:TYR:C	2:D:202:ILE:HD13	2.40	0.47
2:D:166:LEU:HA	4:D:403:HOH:O	2.14	0.47
1:A:429:ASP:HB3	1:A:432:ASP:OD1	2.15	0.46
2:D:157:VAL:HG22	2:D:207:HIS:CD2	2.49	0.46
1:A:247:GLN:N	1:A:247:GLN:OE1	2.49	0.46
1:A:402:TYR:CG	1:A:403:PRO:HA	2.51	0.46
1:A:36:TRP:O	1:A:48:VAL:HG22	2.15	0.46
2:D:104:GLU:O	2:D:104:GLU:CG	2.65	0.45
2:B:126:PRO:HB3	2:B:152:TYR:HB3	1.98	0.45
1:C:172:ALA:CB	1:C:176:VAL:CG2	2.95	0.45
1:C:226:GLN:HB3	1:C:227:PRO:HD2	1.99	0.45
1:A:15:GLY:HA2	1:A:85:SER:HA	1.97	0.45
1:C:36:TRP:O	1:C:48:VAL:HG22	2.17	0.45
1:A:420:ASN:N	1:A:420:ASN:OD1	2.50	0.45
1:C:38:ARG:HD3	1:C:48:VAL:HG11	1.99	0.45
1:C:179:ALA:HB1	1:C:238:HIS:CD2	2.52	0.45
1:C:453:VAL:HG22	1:C:472:ASN:OD1	2.17	0.45
1:C:392:ALA:HB3	1:C:443:LEU:O	2.17	0.45
1:C:176:VAL:HG12	1:C:239:TYR:HB3	1.98	0.44
2:D:104:GLU:O	2:D:104:GLU:HG3	2.17	0.44
1:C:197:SER:O	1:C:198:ALA:C	2.60	0.44
2:B:202:ILE:HG12	2:B:217:ARG:HG2	1.99	0.44
1:C:158:LEU:C	1:C:158:LEU:HD12	2.42	0.44
1:C:412:VAL:HG13	1:C:454:TYR:CE2	2.52	0.44
2:B:133:PRO:HD3	2:B:218:VAL:HG12	2.00	0.44
1:C:384:ASP:HA	1:C:387:LEU:HD12	1.99	0.44
1:A:240:THR:CA	4:A:631:HOH:O	2.66	0.44
1:C:402:TYR:CG	1:C:403:PRO:HA	2.53	0.44
1:C:30:LYS:HE3	1:C:74:THR:HG21	2.00	0.43
1:C:340:LEU:HD23	1:C:368:ILE:HD13	1.99	0.43
1:C:398:LEU:HD12	1:C:398:LEU:N	2.32	0.43
1:A:119:SER:O	1:A:119:SER:OG	2.33	0.43
1:A:177:ASN:OD1	1:A:177:ASN:C	2.61	0.43
1:A:182:TRP:HB2	1:A:195:ILE:HB	2.00	0.43
1:C:176:VAL:HG11	1:C:237:GLN:HB2	2.01	0.43
1:C:2:VAL:HG13	1:C:2:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:GLU:O	2:D:104:GLU:HG2	2.18	0.43
1:C:89:GLU:O	1:C:89:GLU:HG2	2.18	0.43
1:C:219:THR:HG22	1:C:221:THR:HG23	2.00	0.43
1:C:29:ILE:HD12	1:C:53:PRO:HG3	1.99	0.43
2:D:208:LYS:N	2:D:209:PRO:CD	2.82	0.43
1:C:195:ILE:HD12	1:C:211:GLY:HA3	1.99	0.42
1:C:382:PRO:HD3	1:C:394:VAL:HG22	2.00	0.42
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.54	0.42
1:A:149:ILE:HD12	1:A:240:THR:CG2	2.47	0.42
1:A:385:GLU:O	1:A:388:LYS:HB2	2.19	0.42
3:A:501:EDO:C1	4:A:612:HOH:O	2.66	0.42
1:A:60:TYR:CE1	1:A:70:ILE:HG22	2.54	0.42
1:C:108:ASP:OD1	1:C:108:ASP:N	2.50	0.42
1:C:441:LEU:HD21	1:C:443:LEU:CD1	2.49	0.42
1:C:55:ASN:ND2	1:C:57:TYR:HB2	2.34	0.42
1:C:98:ARG:NH1	1:C:109:TYR:CD1	2.88	0.42
1:C:180:VAL:HG21	1:C:218:PHE:CZ	2.55	0.42
1:C:197:SER:O	1:C:199:SER:N	2.53	0.42
1:A:158:LEU:HD23	1:A:158:LEU:C	2.45	0.42
1:A:387:LEU:HD22	1:A:445:LYS:HG3	2.01	0.42
1:C:159:SER:HB3	1:C:254:LYS:HA	2.01	0.41
1:A:107:MET:HG3	4:A:602:HOH:O	2.20	0.41
1:A:398:LEU:HD21	1:A:458:VAL:HG13	2.01	0.41
2:D:185:LEU:HD12	2:D:185:LEU:C	2.45	0.41
1:A:17:SER:HA	1:A:83:MET:O	2.20	0.41
1:A:42:GLY:H	3:A:504:EDO:H22	1.85	0.41
1:A:179:ALA:HA	1:A:238:HIS:NE2	2.36	0.41
1:A:412:VAL:HG12	1:A:417:GLN:CD	2.46	0.41
2:D:144:ALA:H	3:D:301:EDO:H22	1.85	0.41
2:B:81:MET:HE1	2:B:94:TYR:CD2	2.56	0.41
2:D:219:GLU:HB3	2:D:220:PRO:HD2	2.03	0.41
1:A:60:TYR:CZ	1:A:70:ILE:HG22	2.55	0.41
1:C:238:HIS:CD2	1:C:238:HIS:H	2.38	0.41
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.55	0.41
2:B:158:THR:OG1	2:B:206:ASN:HB3	2.21	0.41
1:C:44:GLY:HA3	4:C:651:HOH:O	2.20	0.41
1:C:55:ASN:HD21	1:C:57:TYR:HB2	1.86	0.40
1:C:149:ILE:HD12	1:C:240:THR:CG2	2.47	0.40
2:B:36:TRP:O	2:B:48:MET:HG3	2.21	0.40
1:C:174:GLN:C	4:C:630:HOH:O	2.64	0.40
2:D:126:PRO:HD2	2:D:212:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ARG:NH1	4:A:613:HOH:O	2.33	0.40
2:D:4:LEU:HD23	2:D:96:CYS:SG	2.61	0.40
1:A:105:TYR:CD2	1:A:238:HIS:O	2.72	0.40
2:B:102:TYR:CD2	2:B:103:GLU:CG	3.05	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:SER:OG	2:D:103:GLU:OE1[1_554]	1.97	0.23
1:A:30:LYS:NZ	3:C:502:EDO:O1[1_455]	2.06	0.14
1:A:431:LYS:NZ	2:D:3:GLN:OE1[1_554]	2.12	0.08
2:B:1:GLN:O	1:C:431:LYS:NZ[1_454]	2.15	0.05
1:A:431:LYS:HZ2	2:D:3:GLN:OE1[1_554]	1.56	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/469 (93%)	417 (96%)	18 (4%)	1 (0%)	43	51
1	C	444/469 (95%)	427 (96%)	16 (4%)	1 (0%)	43	51
2	B	211/223 (95%)	209 (99%)	2 (1%)	0	100	100
2	D	212/223 (95%)	208 (98%)	4 (2%)	0	100	100
All	All	1303/1384 (94%)	1261 (97%)	40 (3%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	C	177	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/388 (98%)	377 (99%)	4 (1%)	68	81
1	C	388/388 (100%)	376 (97%)	12 (3%)	35	48
2	B	183/190 (96%)	177 (97%)	6 (3%)	33	45
2	D	185/190 (97%)	180 (97%)	5 (3%)	39	53
All	All	1137/1156 (98%)	1110 (98%)	27 (2%)	44	58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
1	A	176	VAL
1	A	197	SER
1	A	217	ASP
2	B	3	GLN
2	B	48	MET
2	B	50	HIS
2	B	87	ARG
2	B	179	SER
2	B	218	VAL
1	C	54	THR
1	C	89	GLU
1	C	99	TRP
1	C	174	GLN
1	C	176	VAL
1	C	177	ASN
1	C	178	THR
1	C	195	ILE
1	C	197	SER
1	C	216	THR
1	C	420	ASN
1	C	449	GLU
2	D	168[A]	SER
2	D	168[B]	SER

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Mol	Chain	Res	Type
2	D	180	SER
2	D	208	LYS
2	D	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	341	GLN
1	A	351	GLN
1	A	451	HIS
2	B	101	ASN
1	C	55	ASN
1	C	399	ASN
1	C	400	ASN
1	C	414	ASN
2	D	50	HIS
2	D	101	ASN
2	D	171	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	D	302	-	3,3,3	0.44	0	2,2,2	0.49	0
3	EDO	A	504	-	3,3,3	0.53	0	2,2,2	0.45	0
3	EDO	C	503	-	3,3,3	0.47	0	2,2,2	0.53	0
3	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.45	0
3	EDO	C	501	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	C	502	-	3,3,3	0.51	0	2,2,2	0.80	0
3	EDO	D	301	-	3,3,3	0.49	0	2,2,2	0.47	0
3	EDO	A	505	-	3,3,3	0.62	0	2,2,2	0.43	0
3	EDO	C	504	-	3,3,3	0.55	0	2,2,2	0.47	0
3	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.68	0
3	EDO	A	501	-	3,3,3	0.50	0	2,2,2	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	C	501	-	-	0/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	D	301	-	-	1/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	A	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EDO	O1-C1-C2-O2
3	D	301	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	EDO	1	0
3	A	502	EDO	1	0
3	C	502	EDO	1	1
3	D	301	EDO	1	0
3	A	501	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/469 (94%)	0.15	4 (0%) 81 79	31, 64, 95, 120	0
1	C	443/469 (94%)	0.16	7 (1%) 70 67	26, 60, 100, 113	5 (1%)
2	B	215/223 (96%)	0.10	5 (2%) 61 58	29, 54, 100, 132	0
2	D	213/223 (95%)	0.11	5 (2%) 61 58	30, 57, 99, 125	3 (1%)
All	All	1313/1384 (94%)	0.14	21 (1%) 70 67	26, 60, 99, 132	8 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	218	VAL	4.1
2	B	102	TYR	3.0
2	D	220	PRO	2.9
1	C	105	TYR	2.8
1	C	176	VAL	2.7
2	B	218	VAL	2.6
2	B	141	GLY	2.5
1	C	104	PHE	2.5
2	D	203	CYS	2.4
1	A	104	PHE	2.3
2	D	197	GLY	2.3
1	A	99	TRP	2.3
2	B	198	THR	2.2
1	C	84[A]	ASN	2.2
1	C	196	TYR	2.2
2	D	102	TYR	2.1
1	C	182	TRP	2.1
1	C	57	TYR	2.1
1	A	198	ALA	2.1
1	A	85	SER	2.0
2	B	134	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	503	4/4	0.53	0.28	151,268,330,330	0
3	EDO	C	503	4/4	0.59	0.30	103,181,231,231	0
3	EDO	C	502	4/4	0.61	0.34	114,182,284,284	0
3	EDO	D	302	4/4	0.76	0.23	79,107,143,143	0
3	EDO	D	301	4/4	0.78	0.12	76,91,98,102	0
3	EDO	A	505	4/4	0.81	0.15	43,53,64,77	0
3	EDO	A	502	4/4	0.83	0.28	71,99,130,130	0
3	EDO	A	504	4/4	0.84	0.16	43,52,62,64	0
3	EDO	C	504	4/4	0.85	0.19	79,112,143,143	0
3	EDO	C	501	4/4	0.88	0.18	71,86,94,99	0
3	EDO	A	501	4/4	0.92	0.08	56,67,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.