Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 03:07 AM EDT

PDB ID	:	7LR3
Title	:	Complex of Fab 2/6.14 with domain 3 of P. berghei HAP2
Authors	:	Feng, J.; Dong, X.C.; Lu, C.F.; Springer, T.A.
Deposited on	:	2021-02-15
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

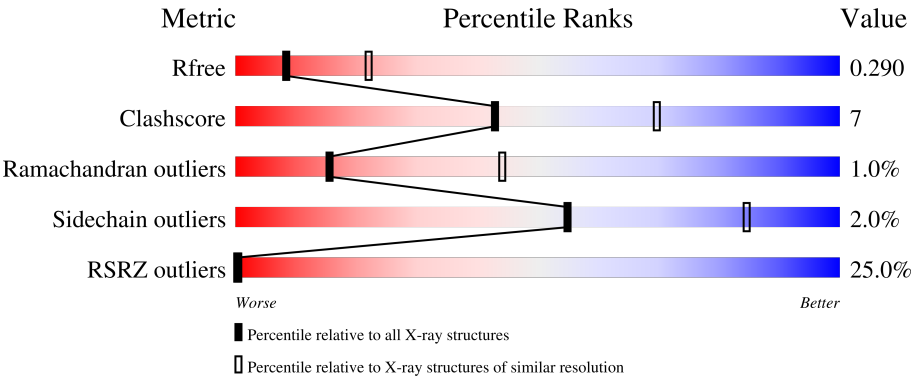
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	B	213	30% 81% 16% ••
1	L	213	19% 79% 18% ••
2	A	228	29% 68% 23% • 6%
2	H	228	11% 72% 18% • 8%
3	D	123	11% 76% 12% • 11%

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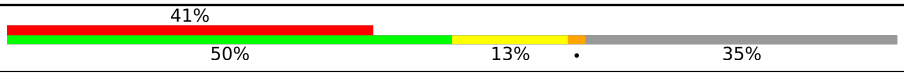
Mol	Chain	Length	Quality of chain
4	C	123	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10350 atoms, of which 0 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 D3_2/6.14 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1638	1029	273	330	6			
1	B	209	Total	C	N	O	S	0	107	0
			2468	1558	411	490	9			

- Molecule 2 is a protein called D3_2/6.14 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	0	0	0
			1580	1004	254	313	9			
2	A	214	Total	C	N	O	S	0	118	0
			2517	1590	410	501	16			

- Molecule 3 is a protein called Hapless 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	110	Total	C	N	O	S	0	0	0
			863	548	143	166	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	516	THR	ASN	engineered mutation	UNP Q4YCF6
D	533	ASN	SER	engineered mutation	UNP Q4YCF6
D	539	GLN	ASN	engineered mutation	UNP Q4YCF6
D	619	HIS	-	expression tag	UNP Q4YCF6
D	620	HIS	-	expression tag	UNP Q4YCF6
D	621	HIS	-	expression tag	UNP Q4YCF6
D	622	HIS	-	expression tag	UNP Q4YCF6
D	623	HIS	-	expression tag	UNP Q4YCF6
D	624	HIS	-	expression tag	UNP Q4YCF6

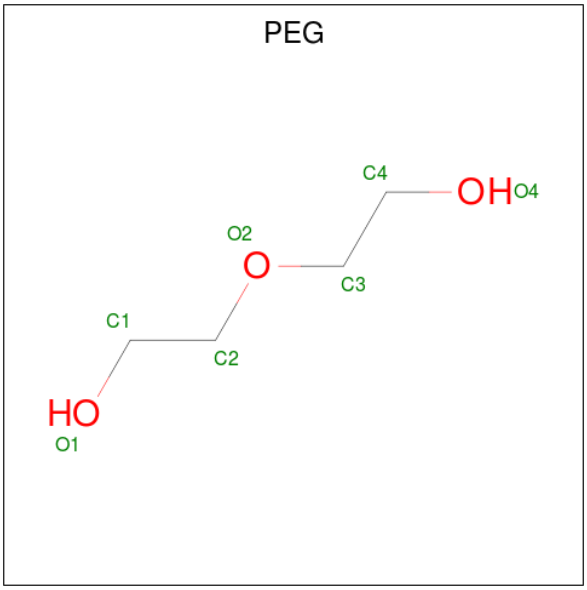
- Molecule 4 is a protein called Hapless 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	80	Total	C	N	O	S	0	80	0
			1244	806	204	224	10			

There are 9 discrepancies between the modelled and reference sequences:

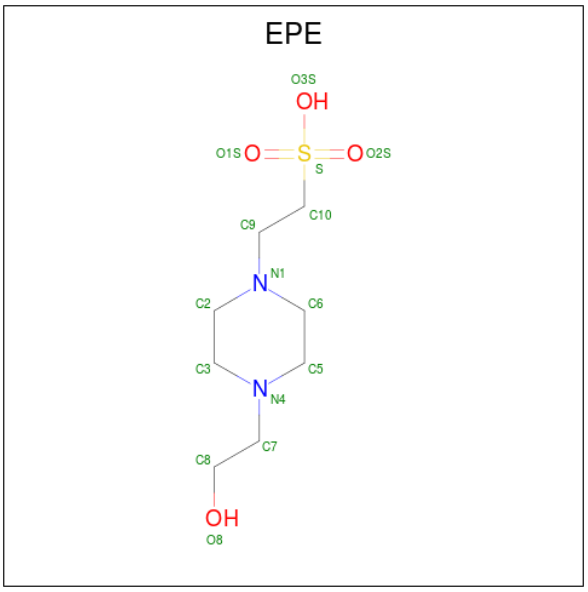
Chain	Residue	Modelled	Actual	Comment	Reference
C	516	THR	ASN	engineered mutation	UNP Q4YCF6
C	533	ASN	SER	engineered mutation	UNP Q4YCF6
C	539	GLN	ASN	engineered mutation	UNP Q4YCF6
C	619	HIS	-	expression tag	UNP Q4YCF6
C	620	HIS	-	expression tag	UNP Q4YCF6
C	621	HIS	-	expression tag	UNP Q4YCF6
C	622	HIS	-	expression tag	UNP Q4YCF6
C	623	HIS	-	expression tag	UNP Q4YCF6
C	624	HIS	-	expression tag	UNP Q4YCF6

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O S 15 8 2 4 1	0	0

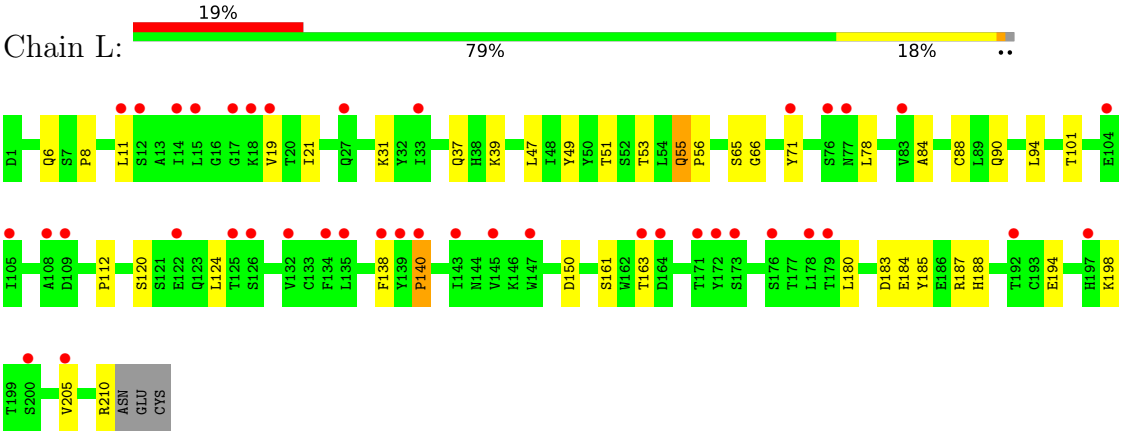
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	6	Total O 6 6	0	0
7	H	7	Total O 7 7	0	0
7	D	5	Total O 5 5	0	0

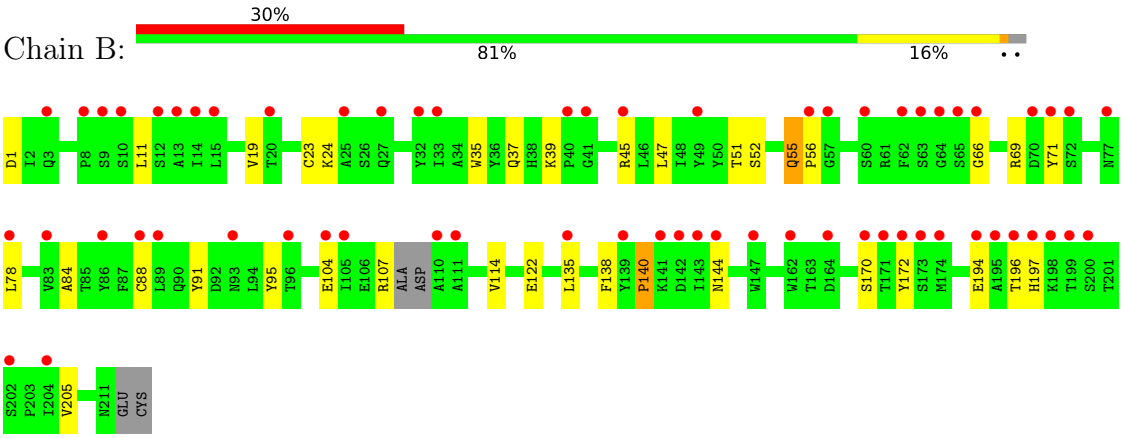
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

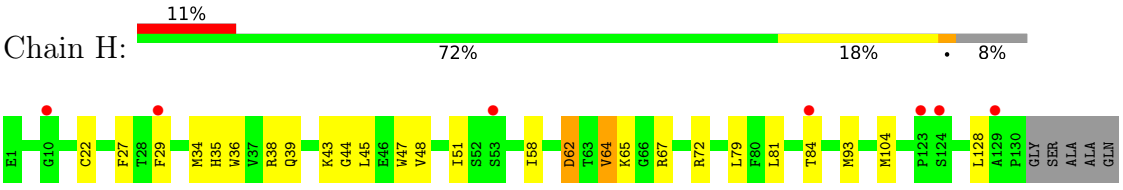
• Molecule 1: D3_2/6.14 Fab light chain

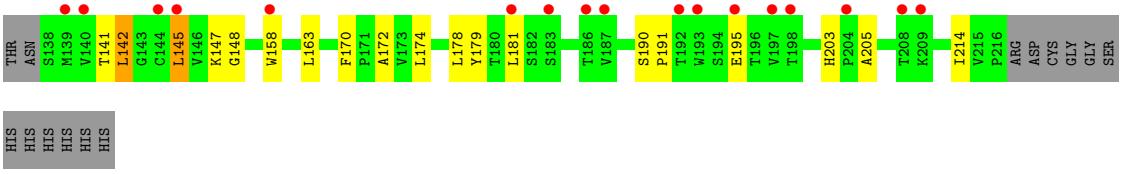


• Molecule 1: D3_2/6.14 Fab light chain

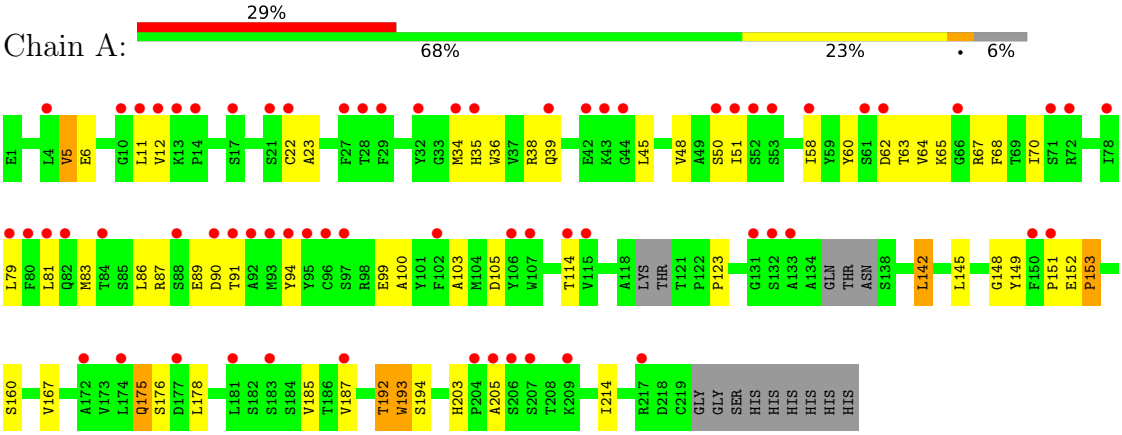


• Molecule 2: D3_2/6.14 Fab heavy chain

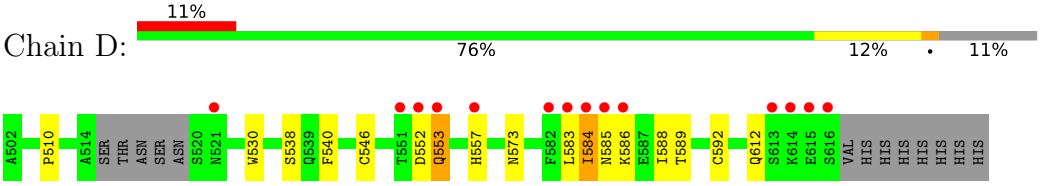




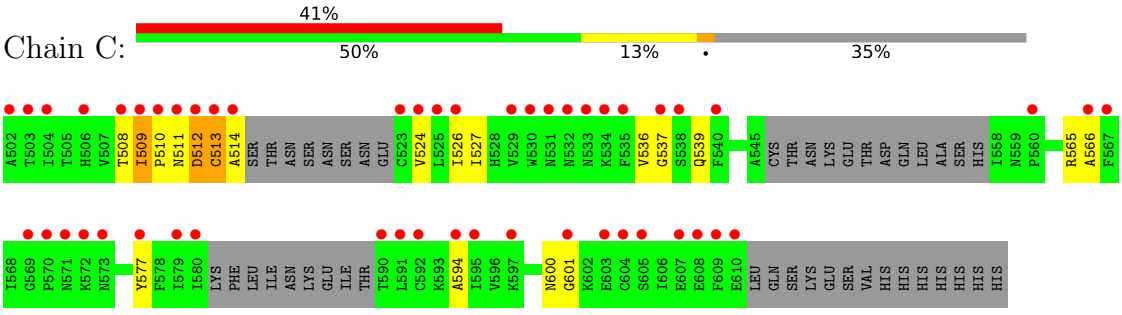
• Molecule 2: D3_2/6.14 Fab heavy chain



• Molecule 3: Hapless 2



• Molecule 4: Hapless 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	78.25Å 122.58Å 168.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.77 – 2.80 49.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.77-2.80) 99.3 (49.57-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.253 , 0.292 0.253 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 83.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10350	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EPE, PEG, CSD

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	B	0.26	0/2528	0.45	0/3427
1	L	0.27	0/1678	0.46	0/2278
2	A	0.26	0/2577	0.46	0/3500
2	H	0.29	0/1621	0.51	0/2211
3	D	0.29	0/871	0.48	0/1179
4	C	0.25	0/1268	0.42	0/1716
All	All	0.27	0/10543	0.46	0/14311

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	2468	0	2382	24	0
1	L	1638	0	1574	23	0
2	A	2517	0	2423	44	0
2	H	1580	0	1540	32	0
3	D	863	0	850	13	0
4	C	1244	0	1226	11	0
5	D	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	15	0	17	2	0
7	D	5	0	0	0	0
7	H	7	0	0	0	0
7	L	6	0	0	0	0
All	All	10350	0	10022	138	0

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 7.

All (138) 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)
2:A:11[B]:LEU:HB2	2:A:151:PRO:HG3	1.62	0.81
2:A:39[B]:GLN:HB2	2:A:45[B]:LEU:HD23	1.72	0.71
2:A:35[A]:HIS:HD1	2:A:50[A]:SER:HG	1.34	0.69
2:A:91[B]:THR:HG23	2:A:114[B]:THR:HA	1.77	0.66
2:A:48[B]:VAL:HG13	2:A:64[B]:VAL:HG21	1.75	0.66
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.78	0.65
2:H:172:ALA:HB2	2:H:181:LEU:HD23	1.79	0.65
3:D:557:HIS:HB3	3:D:583:LEU:HB3	1.79	0.64
2:H:51:ILE:HG22	2:H:58:ILE:HG12	1.80	0.63
2:H:195:GLU:HG3	4:C:600[B]:ASN:HD21	1.63	0.63
1:B:66[B]:GLY:HA3	1:B:71[B]:TYR:HA	1.81	0.63
1:B:144:ASN:HB3	1:B:196:THR:HB	1.80	0.63
2:A:12[B]:VAL:HG11	2:A:86[B]:LEU:HD12	1.81	0.63
1:B:11[B]:LEU:HD13	1:B:19[B]:VAL:HB	1.79	0.63
2:A:175:GLN:OE1	2:A:176:SER:N	2.34	0.61
3:D:546:CYS:HA	3:D:592:CYS:HA	1.81	0.61
2:A:51[B]:ILE:HG22	2:A:58[B]:ILE:HG12	1.83	0.59
2:A:83[A]:MET:HB3	2:A:86[A]:LEU:HD21	1.84	0.59
2:H:51:ILE:HD11	2:H:79:LEU:HD13	1.85	0.59
2:A:5[B]:VAL:HG23	2:A:23[B]:ALA:HB3	1.84	0.59
2:A:22[B]:CYS:HB3	2:A:79[B]:LEU:HB3	1.85	0.58
2:A:48[A]:VAL:HG13	2:A:64[A]:VAL:HG21	1.84	0.58
2:H:67:ARG:O	2:H:84:THR:OG1	2.21	0.58
4:C:565[B]:ARG:NH1	1:B:91[B]:TYR:O	2.36	0.58
1:L:161:SER:HB3	2:H:170:PHE:HB3	1.86	0.56
2:A:22[A]:CYS:HB3	2:A:79[A]:LEU:HB3	1.87	0.56
2:A:148:GLY:HA2	2:A:178:LEU:HB3	1.87	0.56
1:B:37[A]:GLN:HB2	1:B:47[A]:LEU:HD11	1.87	0.56
2:A:63[B]:THR:O	2:A:63[B]:THR:OG1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:66:GLY:HA3	1:L:71:TYR:HA	1.88	0.54
1:L:150:ASP:OD2	1:L:188:HIS:ND1	2.41	0.54
3:D:589:THR:HA	3:D:612:GLN:HA	1.90	0.54
3:D:583:LEU:HG	3:D:584:ILE:HG13	1.90	0.53
2:A:6[B]:GLU:N	2:A:6[B]:GLU:OE1	2.41	0.53
4:C:536[B]:VAL:HG12	4:C:537[B]:GLY:H	1.74	0.52
1:L:194:GLU:HG2	1:L:205:VAL:HG22	1.92	0.52
1:B:114:VAL:HG22	1:B:135:LEU:HG	1.92	0.52
1:B:104[A]:GLU:OE2	1:B:172:TYR:OH	2.27	0.52
1:B:194:GLU:HG2	1:B:205:VAL:HG22	1.91	0.52
2:H:48:VAL:HG13	2:H:64:VAL:HG21	1.92	0.51
4:C:511[A]:ASN:O	4:C:513[A]:CYS:N	2.43	0.51
2:A:6[A]:GLU:HA	2:A:22[A]:CYS:HA	1.92	0.50
2:A:203:HIS:CE1	2:A:205:ALA:HB3	2.47	0.50
3:D:538:SER:HB2	3:D:540:PHE:CE1	2.45	0.50
3:D:584:ILE:HG22	3:D:585:ASN:H	1.76	0.50
2:A:167:VAL:HG22	2:A:185:VAL:HB	1.93	0.50
2:A:193:TRP:HZ2	2:A:214:ILE:HG22	1.76	0.49
1:B:55[B]:GLN:HG2	1:B:56[B]:PRO:HD2	1.93	0.49
1:L:6:GLN:HE21	1:L:21:ILE:HG21	1.78	0.49
1:L:55:GLN:HG2	1:L:56:PRO:HD2	1.93	0.49
1:L:19:VAL:HG13	1:L:78:LEU:HD11	1.94	0.48
2:A:5[A]:VAL:HG23	2:A:23[A]:ALA:HB3	1.96	0.48
2:A:51[A]:ILE:HG22	2:A:58[A]:ILE:HG12	1.93	0.48
1:B:37[B]:GLN:HB2	1:B:47[B]:LEU:HD11	1.96	0.48
2:H:172:ALA:HA	2:H:181:LEU:HB3	1.96	0.47
2:H:43:LYS:HG2	2:H:44:GLY:N	2.30	0.47
2:A:38[A]:ARG:HD3	2:A:94[A]:TYR:CZ	2.50	0.47
1:B:55[A]:GLN:HG2	1:B:56[A]:PRO:HD2	1.96	0.47
1:L:112:PRO:HB3	1:L:138:PHE:CD2	2.50	0.47
2:A:35[A]:HIS:ND1	2:A:50[A]:SER:OG	2.29	0.47
2:H:148:GLY:HA2	2:H:178:LEU:HB3	1.97	0.47
1:L:138:PHE:HD1	1:L:140:PRO:HD3	1.80	0.46
2:A:38[A]:ARG:NH1	2:A:94[A]:TYR:OH	2.46	0.46
2:A:142:LEU:HD13	2:A:214:ILE:HD12	1.97	0.46
2:A:100[A]:ALA:HB3	2:A:105[A]:ASP:HB2	1.98	0.46
1:L:180:LEU:HD12	1:L:184:GLU:OE2	2.15	0.46
3:D:552:ASP:O	3:D:553:GLN:HG2	2.16	0.46
1:B:39[B]:LYS:HG2	1:B:84[B]:ALA:HB2	1.98	0.46
1:L:94:LEU:HD22	2:H:47:TRP:CZ3	2.51	0.45
1:B:122:GLU:OE1	1:B:122:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:SER:OG	2:H:191:PRO:HD3	2.16	0.45
3:D:586:LYS:HD3	3:D:586:LYS:HA	1.67	0.45
2:H:35:HIS:CD2	2:H:104:MET:HG2	2.51	0.45
1:L:8:PRO:O	1:L:101:THR:OG1	2.23	0.45
1:B:24[B]:LYS:HE2	1:B:69[B]:ARG:HH21	1.82	0.45
2:H:27:PHE:HA	2:A:160:SER:HB2	1.98	0.45
2:H:43:LYS:HG2	2:H:44:GLY:H	1.82	0.45
1:L:31:LYS:O	1:L:51:THR:HG23	2.16	0.45
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.99	0.45
2:A:34[B]:MET:HB3	2:A:79[B]:LEU:HD22	1.99	0.45
2:A:36[B]:TRP:HD1	2:A:70[B]:ILE:HD12	1.82	0.45
1:B:138:PHE:HD2	1:B:140:PRO:HD3	1.82	0.45
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.99	0.44
2:A:64[A]:VAL:HG13	2:A:68[A]:PHE:HB2	1.99	0.44
2:A:152:GLU:HA	2:A:153:PRO:HA	1.83	0.44
2:A:39[A]:GLN:HB2	2:A:45[A]:LEU:HD23	1.98	0.44
1:B:19[B]:VAL:HG13	1:B:78[B]:LEU:HD11	1.99	0.44
1:B:140:PRO:HB3	1:B:197:HIS:CE1	2.51	0.44
2:H:22:CYS:N	2:H:79:LEU:O	2.51	0.44
2:H:174:LEU:HD12	2:H:179:TYR:CZ	2.53	0.44
4:C:601[B]:GLY:HA3	2:A:99[B]:GLU:OE1	2.18	0.44
4:C:508[B]:THR:O	4:C:526[B]:ILE:HB	2.18	0.44
2:H:62:ASP:HA	2:H:65:LYS:HE3	1.99	0.44
2:H:145:LEU:HD22	2:H:147:LYS:HB2	1.99	0.43
1:B:23[B]:CYS:HB2	1:B:35[B]:TRP:CH2	2.54	0.43
3:D:538:SER:OG	2:A:194:SER:HB3	2.18	0.43
3:D:589:THR:HG23	3:D:612:GLN:HG2	2.00	0.43
4:C:539[A]:GLN:HG3	4:C:566[A]:ALA:O	2.19	0.43
1:L:120:SER:O	1:L:124:LEU:HG	2.19	0.43
2:H:142:LEU:HD13	2:H:214:ILE:HD12	2.01	0.43
4:C:512[B]:ASP:O	4:C:514[B]:ALA:N	2.52	0.43
2:A:103[B]:ALA:HA	1:B:95[B]:TYR:HE2	1.83	0.43
2:A:142:LEU:HD22	2:A:214:ILE:HG21	2.01	0.43
1:L:183:ASP:O	1:L:187:ARG:HG3	2.19	0.43
2:H:38:ARG:HA	2:H:93:MET:O	2.19	0.43
2:H:51:ILE:HD12	2:H:72:ARG:NE	2.33	0.42
2:A:36[A]:TRP:CD2	2:A:81[A]:LEU:HD22	2.53	0.42
3:D:530:TRP:CE2	6:D:702:EPE:H52	2.54	0.42
1:L:65:SER:OG	1:L:66:GLY:N	2.52	0.42
1:L:198:LYS:HE3	1:L:198:LYS:HB2	1.88	0.42
4:C:527[B]:ILE:HD12	4:C:594[B]:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:187:VAL:HB	2:A:192:THR:HG21	2.01	0.42
3:D:586:LYS:HB3	3:D:588:ILE:HG13	2.01	0.42
2:A:67[A]:ARG:NH1	2:A:90[A]:ASP:OD2	2.52	0.42
2:A:123:PRO:HB3	2:A:149:TYR:HB3	2.01	0.42
4:C:524[B]:VAL:HG22	4:C:577[B]:TYR:HB2	2.01	0.42
2:H:27:PHE:CE2	2:H:29:PHE:HA	2.54	0.42
1:B:11[A]:LEU:HD23	1:B:11[A]:LEU:HA	1.93	0.42
1:B:37[B]:GLN:O	1:B:45[B]:ARG:N	2.51	0.41
2:H:128:LEU:HD21	2:H:145:LEU:HB2	2.02	0.41
2:A:89[B]:GLU:H	2:A:89[B]:GLU:HG3	1.69	0.41
1:L:39:LYS:HG2	1:L:84:ALA:HB2	2.02	0.41
2:H:158:TRP:HB2	2:H:163:LEU:HB2	2.01	0.41
2:A:62[B]:ASP:HA	2:A:65[B]:LYS:HE3	2.02	0.41
2:A:60[A]:TYR:CZ	2:A:70[A]:ILE:HG22	2.56	0.41
1:B:66[A]:GLY:HA3	1:B:71[A]:TYR:HA	2.03	0.41
3:D:573:ASN:HD21	6:D:702:EPE:C3	2.34	0.41
1:L:49:TYR:O	1:L:53:THR:HB	2.21	0.41
2:H:67:ARG:HB3	2:H:84:THR:O	2.21	0.41
2:H:142:LEU:HD22	2:H:214:ILE:HG21	2.01	0.41
2:H:36:TRP:NE1	2:H:81:LEU:HB2	2.36	0.41
1:L:11:LEU:HD13	1:L:19:VAL:HB	2.02	0.40
1:L:163:THR:HG23	2:H:170:PHE:CD1	2.55	0.40
2:H:203:HIS:CE1	2:H:205:ALA:HB3	2.55	0.40
4:C:509[A]:ILE:HG21	4:C:513[A]:CYS:HB2	2.02	0.40
1:B:107[A]:ARG:HD2	1:B:170:SER:HB2	2.03	0.40
1:L:185:TYR:CZ	1:L:210:ARG:HD3	2.57	0.40
1:B:51[B]:THR:O	1:B:52[B]:SER:OG	2.29	0.40

There are no symmetry-related clashes.

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	B	310/213 (146%)	284 (92%)	25 (8%)	1 (0%)	41 72
1	L	208/213 (98%)	192 (92%)	15 (7%)	1 (0%)	29 61
2	A	324/228 (142%)	286 (88%)	37 (11%)	1 (0%)	41 72
2	H	205/228 (90%)	191 (93%)	14 (7%)	0	100 100
3	D	105/123 (85%)	98 (93%)	4 (4%)	3 (3%)	4 15
4	C	144/123 (117%)	118 (82%)	18 (12%)	8 (6%)	2 5
All	All	1296/1128 (115%)	1169 (90%)	113 (9%)	14 (1%)	15 41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	584	ILE
4	C	510[A]	PRO
4	C	510[B]	PRO
4	C	512[A]	ASP
4	C	512[B]	ASP
1	L	140	PRO
3	D	510	PRO
4	C	509[A]	ILE
4	C	509[B]	ILE
4	C	513[A]	CYS
4	C	513[B]	CYS
1	B	140	PRO
3	D	553	GLN
2	A	153	PRO

5.3.2 Protein sidechains (i)

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	B	278/189 (147%)	272 (98%)	6 (2%)	52 83
1	L	186/189 (98%)	183 (98%)	3 (2%)	62 88
2	A	281/195 (144%)	272 (97%)	9 (3%)	39 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	181/195 (93%)	176 (97%)	5 (3%)	43 77
3	D	98/111 (88%)	98 (100%)	0	100 100
4	C	140/112 (125%)	140 (100%)	0	100 100
All	All	1164/991 (118%)	1141 (98%)	23 (2%)	55 84

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	55	GLN
1	L	88	CYS
1	L	90	GLN
2	H	62	ASP
2	H	64	VAL
2	H	141	THR
2	H	142	LEU
2	H	145	LEU
2	A	5[A]	VAL
2	A	5[B]	VAL
2	A	87[A]	ARG
2	A	87[B]	ARG
2	A	142	LEU
2	A	145	LEU
2	A	175	GLN
2	A	192	THR
2	A	193	TRP
1	B	1[A]	ASP
1	B	1[B]	ASP
1	B	55[A]	GLN
1	B	55[B]	GLN
1	B	88[A]	CYS
1	B	88[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	573	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is 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	CSD	D	604	3	3,7,8	0.95	0	1,8,10	0.85	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	CSD	D	604	3	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	604	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
5	PEG	D	701	-	6,6,6	0.50	0	5,5,5	0.23	0
6	EPE	D	702	-	15,15,15	0.83	1 (6%)	18,20,20	1.74	5 (27%)

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
5	PEG	D	701	-	-	0/4/4/4	-
6	EPE	D	702	-	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	702	EPE	C10-S	2.77	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	702	EPE	C5-N4-C3	3.74	117.25	108.83
6	D	702	EPE	C7-N4-C5	2.79	118.36	111.23
6	D	702	EPE	C7-N4-C3	2.65	118.02	111.23
6	D	702	EPE	O3S-S-C10	2.57	109.92	105.77
6	D	702	EPE	O2S-S-C10	2.40	109.80	106.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	702	EPE	C8-C7-N4-C3
6	D	702	EPE	S-C10-C9-N1
6	D	702	EPE	N4-C7-C8-O8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	702	EPE	2	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	B	209/213 (98%)	1.61	63 (30%)	0 0	66, 127, 194, 312	0
1	L	210/213 (98%)	1.15	41 (19%)	1 0	90, 155, 212, 234	0
2	A	214/228 (93%)	1.64	66 (30%)	0 0	69, 122, 194, 311	0
2	H	209/228 (91%)	0.84	24 (11%)	4 2	79, 133, 199, 292	0
3	D	109/123 (88%)	0.75	14 (12%)	3 2	58, 99, 246, 296	0
4	C	80/123 (65%)	3.08	50 (62%)	0 0	82, 134, 236, 265	0
All	All	1031/1128 (91%)	1.39	258 (25%)	0 0	58, 133, 212, 312	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	C	523[A]	CYS	21.8
1	L	171	THR	12.7
3	D	615	GLU	8.8
2	A	205	ALA	8.7
1	B	139	TYR	7.9
4	C	503[A]	THR	7.8
3	D	613	SER	7.6
1	B	173	SER	7.2
2	H	192	THR	6.8
4	C	580[A]	ILE	6.8
1	B	110	ALA	6.8
3	D	585	ASN	6.8
2	A	53[A]	SER	6.5
1	L	163	THR	6.5
2	A	17[A]	SER	6.4
1	B	171	THR	6.3
4	C	610[A]	GLU	6.3
2	A	78[A]	ILE	6.2
2	A	132	SER	6.1

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Mol	Chain	Res	Type	RSRZ
4	C	509[A]	ILE	6.1
2	A	133	ALA	6.1
1	B	143	ILE	6.0
1	B	13[A]	ALA	6.0
1	B	14[A]	ILE	5.8
1	B	77[A]	ASN	5.8
1	B	15[A]	LEU	5.7
3	D	616	SER	5.7
1	B	135	LEU	5.6
1	B	199	THR	5.5
4	C	502[A]	ALA	5.5
4	C	579[A]	ILE	5.5
4	C	510[A]	PRO	5.5
4	C	511[A]	ASN	5.4
4	C	573[A]	ASN	5.4
4	C	534[A]	LYS	5.4
2	H	198	THR	5.3
2	A	81[A]	LEU	5.3
3	D	614	LYS	5.2
1	B	141	LYS	5.2
3	D	552	ASP	5.2
1	L	77	ASN	5.1
1	L	15	LEU	5.1
2	A	21[A]	SER	5.0
3	D	521	ASN	5.0
1	L	197	HIS	5.0
2	A	94[A]	TYR	4.9
4	C	594[A]	ALA	4.9
1	L	14	ILE	4.9
1	L	200	SER	4.8
2	A	151	PRO	4.8
4	C	597[A]	LYS	4.8
2	A	10[A]	GLY	4.7
4	C	571[A]	ASN	4.7
2	A	206	SER	4.6
1	L	126	SER	4.6
4	C	566[A]	ALA	4.5
1	L	105	ILE	4.5
2	A	51[A]	ILE	4.5
4	C	590[A]	THR	4.4
4	C	535[A]	PHE	4.4
4	C	572[A]	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
4	C	569[A]	GLY	4.3
4	C	607[A]	GLU	4.3
1	B	170	SER	4.3
1	B	147	TRP	4.2
4	C	530[A]	TRP	4.2
4	C	604[A]	CYS	4.2
1	B	195	ALA	4.1
3	D	584	ILE	4.1
4	C	609[A]	PHE	4.1
4	C	508[A]	THR	4.0
2	A	217	ARG	4.0
4	C	537[A]	GLY	4.0
2	H	193	TRP	4.0
2	A	50[A]	SER	4.0
1	L	109	ASP	4.0
2	H	123	PRO	4.0
2	A	29[A]	PHE	3.9
2	A	131	GLY	3.9
2	A	91[A]	THR	3.9
1	B	174	MET	3.9
2	A	97[A]	SER	3.9
3	D	583	LEU	3.9
1	B	93[A]	ASN	3.8
2	A	183	SER	3.8
1	L	147	TRP	3.8
4	C	577[A]	TYR	3.8
1	L	17	GLY	3.7
4	C	560[A]	PRO	3.7
2	A	106[A]	TYR	3.7
1	L	83	VAL	3.7
2	A	35[A]	HIS	3.7
1	B	172	TYR	3.7
1	B	142	ASP	3.6
2	A	61[A]	SER	3.7
3	D	586	LYS	3.6
1	B	194	GLU	3.6
1	B	204	ILE	3.6
2	A	66[A]	GLY	3.6
2	A	95[A]	TYR	3.6
2	A	11[A]	LEU	3.6
4	C	514[A]	ALA	3.6
2	H	53	SER	3.5

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Mol	Chain	Res	Type	RSRZ
4	C	524[A]	VAL	3.5
1	L	143	ILE	3.5
1	L	104	GLU	3.5
1	L	18	LYS	3.5
2	H	209	LYS	3.5
4	C	608[A]	GLU	3.4
3	D	553	GLN	3.4
2	A	181	LEU	3.4
2	H	208	THR	3.4
2	A	209	LYS	3.4
2	A	28[A]	THR	3.4
2	A	14[A]	PRO	3.4
2	A	115[A]	VAL	3.4
1	L	12	SER	3.3
4	C	591[A]	LEU	3.3
2	A	12[A]	VAL	3.3
4	C	538[A]	SER	3.3
2	A	13[A]	LYS	3.3
4	C	533[A]	ASN	3.3
2	A	150	PHE	3.3
1	B	56[A]	PRO	3.3
2	A	34[A]	MET	3.2
1	B	70[A]	ASP	3.2
1	B	196	THR	3.2
1	L	108	ALA	3.2
1	L	139	TYR	3.2
4	C	601[A]	GLY	3.2
2	A	172	ALA	3.2
1	B	60[A]	SER	3.1
1	B	57[A]	GLY	3.1
2	H	84	THR	3.1
1	L	173	SER	3.1
2	H	187	VAL	3.1
1	B	111	ALA	3.1
1	B	83[A]	VAL	3.1
2	H	195	GLU	3.1
4	C	532[A]	ASN	3.0
2	H	140	VAL	3.0
1	L	19	VAL	3.0
2	A	79[A]	LEU	2.9
2	A	82[A]	GLN	2.9
1	L	178	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	174	LEU	2.9
4	C	512[A]	ASP	2.9
4	C	540[A]	PHE	2.9
1	B	197	HIS	2.9
2	A	44[A]	GLY	2.9
2	A	88[A]	SER	2.9
2	A	43[A]	LYS	2.9
1	B	71[A]	TYR	2.9
1	B	78[A]	LEU	2.9
1	B	8[A]	PRO	2.8
2	A	72[A]	ARG	2.8
2	A	84[A]	THR	2.8
1	B	86[A]	TYR	2.8
2	H	158	TRP	2.8
1	B	200	SER	2.8
2	H	124	SER	2.8
2	A	187	VAL	2.8
4	C	525[A]	LEU	2.8
2	H	129	ALA	2.8
2	A	80[A]	PHE	2.7
2	A	177	ASP	2.7
1	L	122	GLU	2.7
1	L	140	PRO	2.7
1	B	9[A]	SER	2.7
2	H	183	SER	2.7
4	C	526[A]	ILE	2.7
2	A	4[A]	LEU	2.6
2	H	139	MET	2.6
1	B	66[A]	GLY	2.6
1	L	76	SER	2.6
1	B	144	ASN	2.6
2	A	204	PRO	2.6
1	B	198	LYS	2.5
2	A	71[A]	SER	2.5
1	L	205	VAL	2.5
1	B	65[A]	SER	2.5
1	L	192	THR	2.5
2	A	22[A]	CYS	2.5
1	B	41[A]	GLY	2.5
2	A	96[A]	CYS	2.5
4	C	529[A]	VAL	2.5
2	H	181	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	107[A]	TRP	2.5
4	C	513[A]	CYS	2.5
1	B	89[A]	LEU	2.4
1	L	134	PHE	2.4
1	B	162	TRP	2.4
2	A	207	SER	2.4
1	B	10[A]	SER	2.4
2	A	32[A]	TYR	2.4
4	C	531[A]	ASN	2.4
2	H	144	CYS	2.4
2	A	114[A]	THR	2.4
1	B	25[A]	ALA	2.4
2	A	102[A]	PHE	2.3
4	C	504[A]	ILE	2.3
1	B	3[A]	GLN	2.3
1	L	125	THR	2.3
2	H	145	LEU	2.3
2	H	197	VAL	2.3
1	B	40[A]	PRO	2.3
2	A	42[A]	GLU	2.3
1	L	176	SER	2.3
1	B	202	SER	2.3
1	L	138	PHE	2.3
4	C	567[A]	PHE	2.3
1	B	72[A]	SER	2.3
1	B	45[A]	ARG	2.3
1	B	96[A]	THR	2.3
2	A	93[A]	MET	2.2
1	L	172	TYR	2.2
2	A	27[A]	PHE	2.2
4	C	595[A]	ILE	2.2
1	L	27	GLN	2.2
4	C	506[A]	HIS	2.2
2	A	58[A]	ILE	2.2
1	L	164	ASP	2.2
1	B	105[A]	ILE	2.2
1	B	62[A]	PHE	2.2
3	D	551	THR	2.2
4	C	605[A]	SER	2.2
1	B	49[A]	TYR	2.2
1	B	88[A]	CYS	2.2
2	H	29	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
4	C	603[A]	GLU	2.2
2	H	204	PRO	2.2
1	B	32[A]	TYR	2.2
1	B	164	ASP	2.1
2	A	90[A]	ASP	2.1
2	A	92[A]	ALA	2.1
2	H	10	GLY	2.1
3	D	557	HIS	2.1
2	A	39[A]	GLN	2.1
1	B	104[A]	GLU	2.1
1	L	132	VAL	2.1
1	L	145	VAL	2.1
4	C	570[A]	PRO	2.1
1	B	64[A]	GLY	2.1
1	L	135	LEU	2.1
1	B	12[A]	SER	2.1
1	B	27[A]	GLN	2.0
2	H	186	THR	2.0
3	D	582	PHE	2.0
2	A	52[A]	SER	2.0
1	B	20[A]	THR	2.0
1	L	33	ILE	2.0
1	B	33[A]	ILE	2.0
2	A	62[A]	ASP	2.0
1	L	71	TYR	2.0
1	L	11	LEU	2.0
4	C	592[A]	CYS	2.0
1	B	63[A]	SER	2.0
1	L	179	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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(Å^2)	Q<0.9
3	CSD	D	604	8/9	0.90	0.22	69,79,101,121	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
5	PEG	D	701	7/7	0.41	0.37	120,137,151,156	0
6	EPE	D	702	15/15	0.72	0.30	89,98,108,109	15

6.5 Other polymers (i)

There are no such residues in this entry.