



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:36 AM UTC

PDB ID : 7LR3 / pdb_00007lr3
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 ⓘ 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:

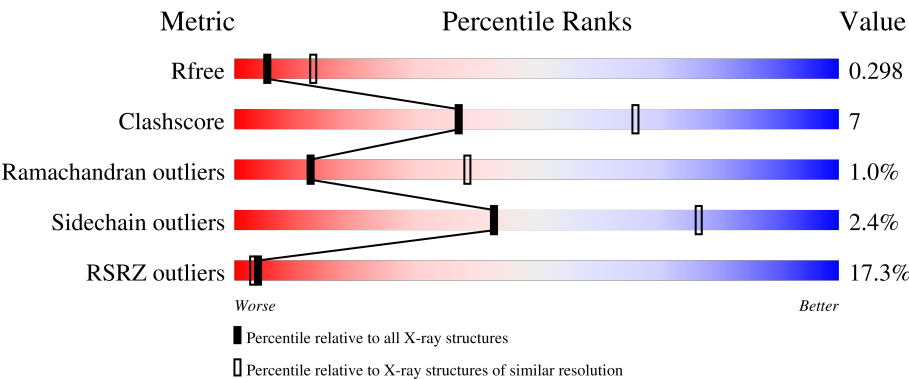
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	B	213	20% 82% 15% ..
1	L	213	6% 79% 19% ..
2	A	228	22% 66% 25% 6%
2	H	228	12% 71% 20% 8%
3	D	123	13% 74% 14% 11%

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Mol	Chain	Length	Quality of chain
4	C	123	23% 48% 14% • 35%

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

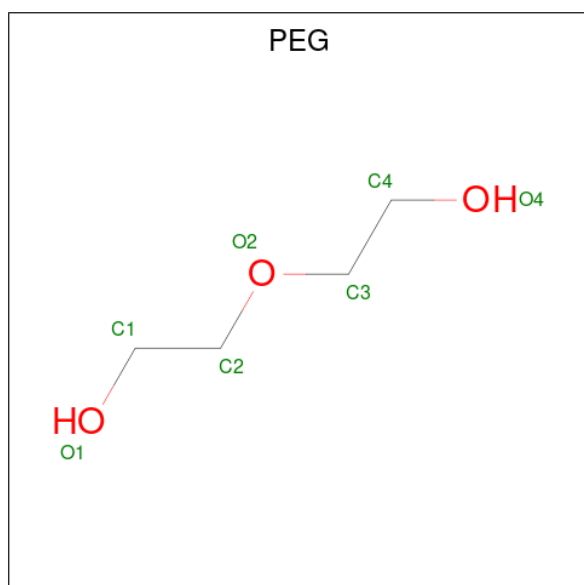
- Molecule 4 is a protein called Hapless 2.

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:

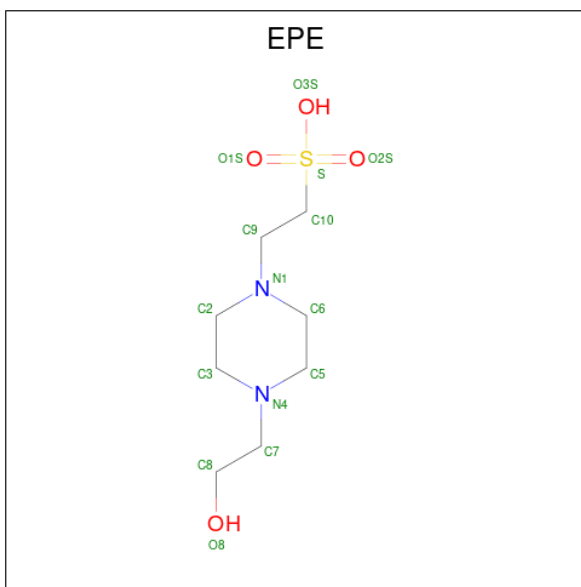
Chain	Residue	Modelled	Actual	Comment	Reference
C	516	THR	ASN	engineered mutation	UNP Q4YCF6
C	533	ASN	SER	engineered mutation	UNP Q4YCF6
C	539	GLN	ASN	engineered mutation	UNP Q4YCF6
C	619	HIS	-	expression tag	UNP Q4YCF6
C	620	HIS	-	expression tag	UNP Q4YCF6
C	621	HIS	-	expression tag	UNP Q4YCF6
C	622	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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



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 (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

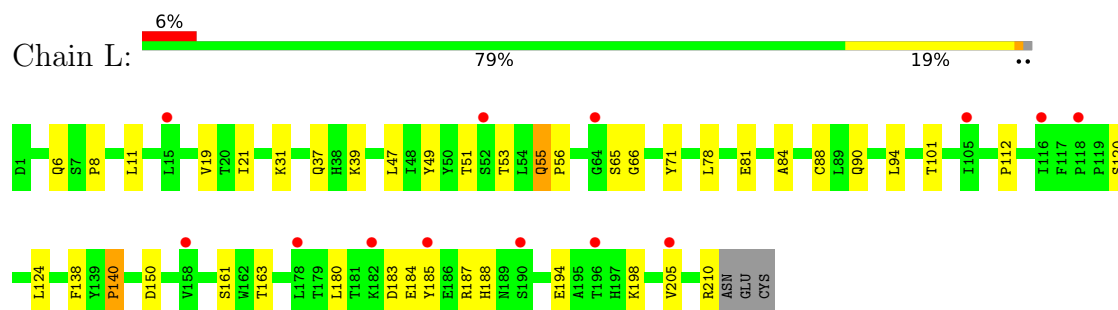
- Molecule 7 is water.

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

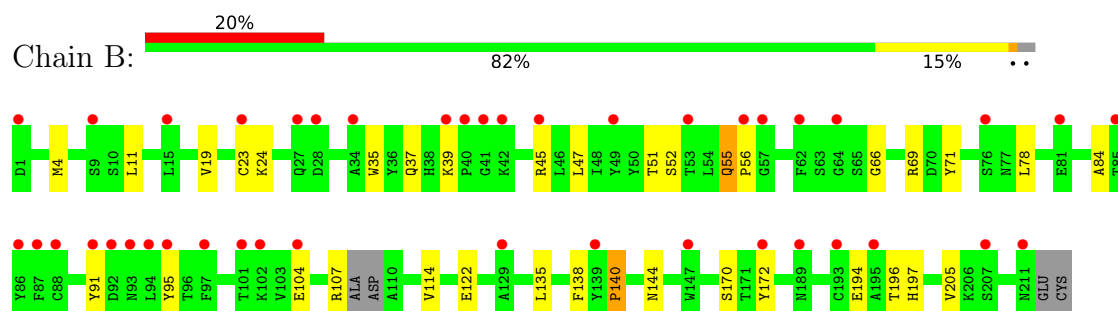
3 Residue-property plots [i](#)

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.

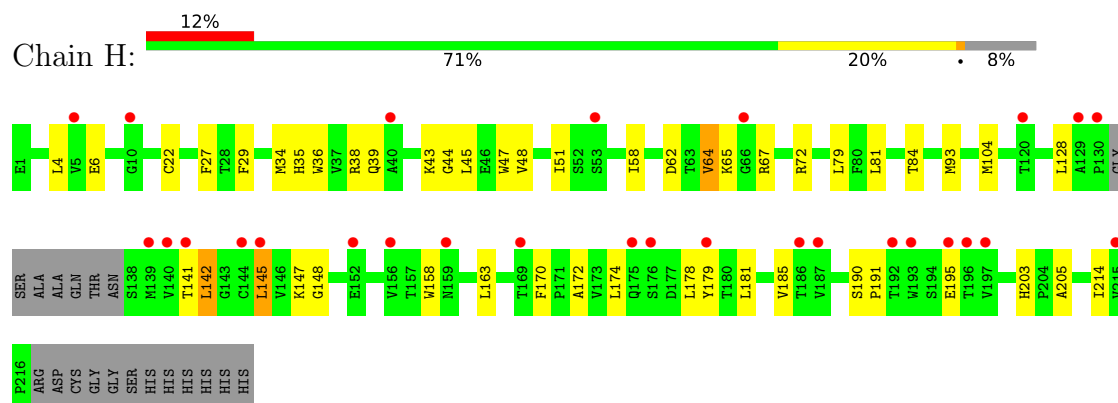
- Molecule 1: D3_2/6.14 Fab light chain



- Molecule 1: D3_2/6.14 Fab light chain

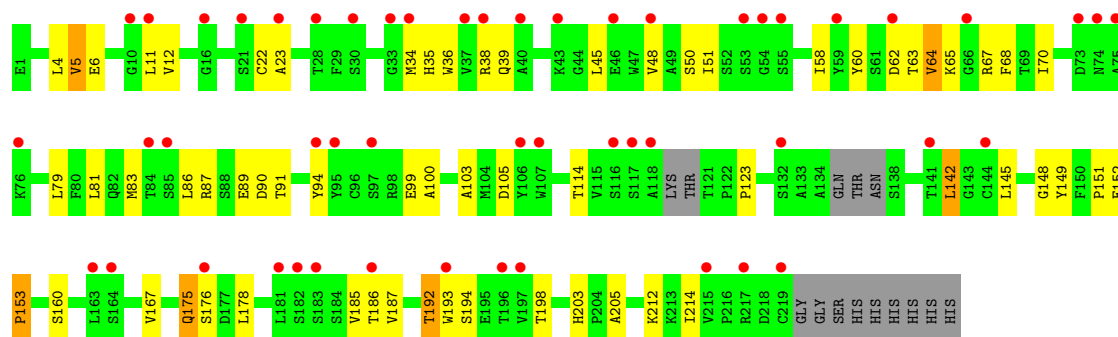


- Molecule 2: D3_2/6.14 Fab heavy chain

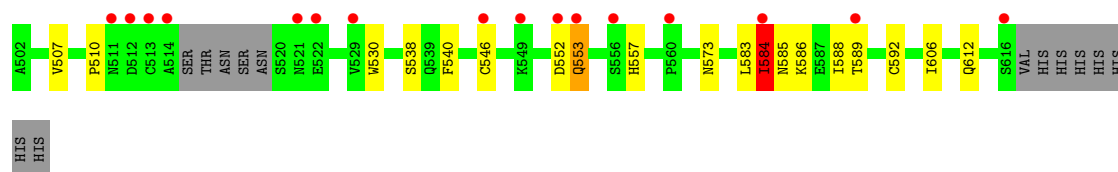


- Molecule 2: D3_2/6.14 Fab heavy chain

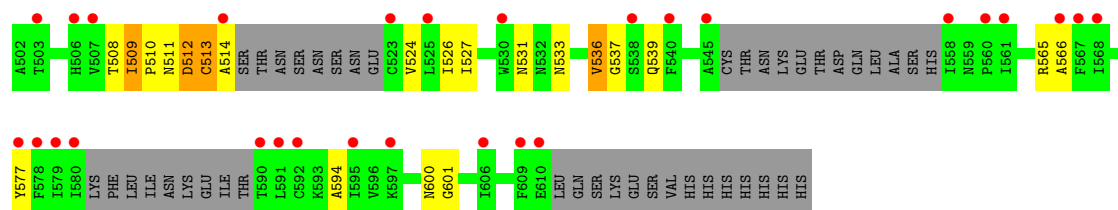




• Molecule 3: Hapless 2



• Molecule 4: Hapless 2



4 Data and refinement statistics

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 42.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.77-2.80) 99.3 (42.77-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.253 , 0.292 0.263 , 0.298	Depositor DCC
R_{free} test set	2000 reflections (3.13%)	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)	0.30 , 137.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, CSD, PEG

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	0.10	0/2528	0.25	0/3427
1	L	0.14	0/1678	0.30	0/2278
2	A	0.10	0/2577	0.26	0/3500
2	H	0.18	0/1621	0.37	0/2211
3	D	0.18	0/871	0.34	0/1179
4	C	0.06	0/1268	0.17	0/1716
All	All	0.13	0/10543	0.28	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 [i](#)

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	25	0
1	L	1638	0	1574	24	0
2	A	2517	0	2423	47	0
2	H	1580	0	1540	33	0
3	D	863	0	850	13	0
4	C	1244	0	1226	12	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	145	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 (145) 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:8:PRO:O	1:L:101:THR:OG1	2.23	0.55
2:H:4:LEU:HD21	2:H:34:MET:HE1	1.87	0.55
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:4[B]:LEU:HD21	2:A:34[B]:MET:HE1	1.94	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:A:83[B]:MET:HE2	2:A:86[B]:LEU:HD21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:B:4[A]:MET:HE3	1:B:23[A]:CYS:SG	2.58	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
4:C:531[A]:ASN:C	4:C:533[A]:ASN:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:39:LYS:NZ	1:L:81:GLU:O	2.39	0.42
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
2:A:198:THR:HG23	2:A:212:LYS:C	2.45	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

5.3.1 Protein backbone

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%)	36	66
1	L	208/213 (98%)	192 (92%)	15 (7%)	1 (0%)	24	55
2	A	324/228 (142%)	286 (88%)	37 (11%)	1 (0%)	36	66
2	H	205/228 (90%)	191 (93%)	14 (7%)	0	100	100
3	D	105/123 (85%)	98 (93%)	4 (4%)	3 (3%)	3	13
4	C	144/123 (117%)	118 (82%)	18 (12%)	8 (6%)	1	4
All	All	1296/1128 (115%)	1169 (90%)	113 (9%)	14 (1%)	12	36

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

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%)	276 (99%)	2 (1%)	76	91
1	L	186/189 (98%)	183 (98%)	3 (2%)	55	83
2	A	281/195 (144%)	270 (96%)	11 (4%)	28	64
2	H	181/195 (93%)	175 (97%)	6 (3%)	33	69
3	D	98/111 (88%)	95 (97%)	3 (3%)	35	70
4	C	140/112 (125%)	138 (99%)	2 (1%)	59	85
All	All	1164/991 (118%)	1137 (98%)	27 (2%)	43	78

All (27) 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	6	GLU
2	H	64	VAL
2	H	141	THR
2	H	142	LEU
2	H	145	LEU
2	H	185	VAL
3	D	507	VAL
3	D	584	ILE
3	D	606	ILE
4	C	536[A]	VAL
4	C	536[B]	VAL
2	A	5[A]	VAL
2	A	5[B]	VAL
2	A	64[A]	VAL
2	A	64[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	186	THR
2	A	192	THR
1	B	55[A]	GLN
1	B	55[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	548	ASN
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	4,7,8	1.13	0	1,8,10	0.84	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 [i](#)

There are no oligosaccharides 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	0.51	0	5,5,5	0.23	0
6	EPE	D	702	-	15,15,15	0.83	1 (6%)	19,20,20	1.62	5 (26%)

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	2.75	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	702	EPE	C5-N4-C3	3.91	117.25	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	702	EPE	C7-N4-C5	2.67	118.36	111.24
6	D	702	EPE	C7-N4-C3	2.54	118.02	111.24
6	D	702	EPE	O2S-S-C10	2.03	109.80	106.73
6	D	702	EPE	O3S-S-C10	2.00	109.92	106.00

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, 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	B	209/213 (98%)	1.10	42 (20%) 3 2	33, 87, 194, 312	107 (51%)
1	L	210/213 (98%)	0.72	13 (6%) 26 20	90, 155, 212, 234	0
2	A	214/228 (93%)	1.31	51 (23%) 2 1	34, 61, 194, 311	118 (55%)
2	H	209/228 (91%)	0.94	28 (13%) 7 5	79, 133, 199, 292	0
3	D	109/123 (88%)	0.99	16 (14%) 6 4	58, 99, 246, 296	0
4	C	80/123 (65%)	1.67	28 (35%) 1 0	41, 67, 118, 132	80 (100%)
All	All	1031/1128 (91%)	1.07	178 (17%) 4 3	33, 127, 207, 312	305 (29%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	C	560[A]	PRO	7.2
2	H	186	THR	6.4
4	C	579[A]	ILE	6.1
1	B	56[A]	PRO	6.0
2	A	117[A]	SER	5.8
4	C	578[A]	PHE	5.8
2	A	94[A]	TYR	5.7
2	A	118[A]	ALA	5.7
2	H	192	THR	5.5
2	A	84[A]	THR	4.3
4	C	540[A]	PHE	4.3
2	A	48[A]	VAL	4.3
4	C	523[A]	CYS	4.1
2	A	219	CYS	4.0
1	B	39[A]	LYS	4.0
2	A	97[A]	SER	3.9
2	A	75[A]	ALA	3.9
4	C	580[A]	ILE	3.8
1	B	94[A]	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	A	181	LEU	3.7
2	H	140	VAL	3.7
4	C	558[A]	ILE	3.6
4	C	525[A]	LEU	3.6
1	B	42[A]	LYS	3.5
2	A	144	CYS	3.5
1	L	185	TYR	3.4
4	C	590[A]	THR	3.4
1	B	95[A]	TYR	3.4
2	A	95[A]	TYR	3.4
2	H	141	THR	3.3
2	A	186	THR	3.3
1	B	81[A]	GLU	3.3
2	H	130	PRO	3.2
1	B	87[A]	PHE	3.2
2	A	34[A]	MET	3.2
1	B	129	ALA	3.2
3	D	514	ALA	3.2
4	C	606[A]	ILE	3.2
1	B	62[A]	PHE	3.2
2	H	187	VAL	3.2
2	H	193	TRP	3.2
3	D	513	CYS	3.1
2	A	62[A]	ASP	3.1
2	A	30[A]	SER	3.1
2	A	85[A]	SER	3.1
4	C	503[A]	THR	3.1
1	B	1[A]	ASP	3.1
1	B	102[A]	LYS	3.1
2	H	169	THR	3.1
2	A	21[A]	SER	3.0
3	D	512	ASP	3.0
3	D	560	PRO	3.0
1	B	92[A]	ASP	3.0
4	C	506[A]	HIS	3.0
1	B	97[A]	PHE	2.9
2	A	217	ARG	2.9
2	A	116[A]	SER	2.9
2	A	11[A]	LEU	2.9
1	B	41[A]	GLY	2.9
2	A	106[A]	TYR	2.9
1	B	85[A]	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	57[A]	GLY	2.9
1	B	93[A]	ASN	2.9
2	H	139	MET	2.8
2	A	40[A]	ALA	2.8
2	A	215	VAL	2.8
1	B	211	ASN	2.8
4	C	610[A]	GLU	2.8
4	C	597[A]	LYS	2.8
2	H	129	ALA	2.8
2	A	54[A]	GLY	2.8
1	B	147	TRP	2.8
1	B	86[A]	TYR	2.8
2	A	73[A]	ASP	2.8
1	L	182	LYS	2.8
4	C	568[A]	ILE	2.7
3	D	521	ASN	2.7
3	D	556	SER	2.7
1	B	64[A]	GLY	2.7
1	B	207	SER	2.7
2	A	55[A]	SER	2.7
1	B	28[A]	ASP	2.7
1	L	52	SER	2.7
2	A	132	SER	2.7
2	A	183	SER	2.7
3	D	616	SER	2.7
2	A	43[A]	LYS	2.6
1	B	45[A]	ARG	2.6
2	H	196	THR	2.6
4	C	595[A]	ILE	2.6
1	B	40[A]	PRO	2.6
1	L	116	ILE	2.6
2	A	38[A]	ARG	2.6
2	A	16[A]	GLY	2.6
3	D	511	ASN	2.6
1	B	49[A]	TYR	2.5
4	C	530[A]	TRP	2.5
2	H	40	ALA	2.5
4	C	514[A]	ALA	2.5
2	A	74[A]	ASN	2.5
4	C	567[A]	PHE	2.5
4	C	566[A]	ALA	2.5
4	C	507[A]	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	193	TRP	2.5
2	H	195	GLU	2.5
1	B	101[A]	THR	2.5
1	B	195	ALA	2.5
2	H	145	LEU	2.4
2	A	176	SER	2.4
1	B	172	TYR	2.4
2	H	179	TYR	2.4
3	D	553	GLN	2.4
2	H	144	CYS	2.4
4	C	592[A]	CYS	2.4
1	B	76[A]	SER	2.4
2	H	175	GLN	2.4
3	D	589	THR	2.4
2	A	37[A]	VAL	2.4
1	B	27[A]	GLN	2.4
2	H	197	VAL	2.3
2	A	182	SER	2.3
1	B	91[A]	TYR	2.3
1	L	64	GLY	2.3
2	A	33[A]	GLY	2.3
2	A	66[A]	GLY	2.3
4	C	609[A]	PHE	2.3
4	C	577[A]	TYR	2.3
2	A	163	LEU	2.3
3	D	584	ILE	2.3
2	A	197	VAL	2.3
2	A	10[A]	GLY	2.3
4	C	591[A]	LEU	2.3
2	A	107[A]	TRP	2.3
4	C	538[A]	SER	2.3
1	B	34[A]	ALA	2.2
1	B	104[A]	GLU	2.2
1	L	105	ILE	2.2
2	A	53[A]	SER	2.2
1	B	193	CYS	2.2
2	A	196	THR	2.2
2	H	152	GLU	2.2
2	A	46[A]	GLU	2.2
1	B	53[A]	THR	2.2
2	H	53	SER	2.2
4	C	561[A]	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	552	ASP	2.2
1	B	9[A]	SER	2.2
2	H	176	SER	2.2
2	A	164	SER	2.2
1	L	15	LEU	2.1
2	A	23[A]	ALA	2.1
2	H	215	VAL	2.1
3	D	529	VAL	2.1
1	L	196	THR	2.1
2	H	10	GLY	2.1
1	B	139	TYR	2.1
4	C	545[A]	ALA	2.1
2	A	28[A]	THR	2.1
2	A	141	THR	2.1
2	A	59[A]	TYR	2.1
2	H	5	VAL	2.1
2	H	156	VAL	2.1
3	D	549	LYS	2.1
1	L	118	PRO	2.1
2	H	159	ASN	2.1
1	L	178	LEU	2.1
2	H	66	GLY	2.1
1	B	23[A]	CYS	2.0
1	B	88[A]	CYS	2.0
2	A	76[A]	LYS	2.0
3	D	546	CYS	2.0
1	L	158	VAL	2.0
1	B	15[A]	LEU	2.0
2	H	120	THR	2.0
3	D	522	GLU	2.0
1	L	190	SER	2.0
1	L	205	VAL	2.0
1	B	189	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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($\text{\AA}^2$)	Q<0.9
3	CSD	D	604	8/9	0.92	0.17	69,79,101,121	0

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($\text{\AA}^2$)	Q<0.9
5	PEG	D	701	7/7	0.80	0.15	120,137,151,156	0
6	EPE	D	702	15/15	0.90	0.16	89,98,108,109	15

6.5 Other polymers [i](#)

There are no such residues in this entry.